Fumaric acid, 2,4,4-trimethylpentyl hept-2-yl ester

Inchi: InChI=1S/C19H34O4/c1-7-8-9-10-16(3)23-18(21)12-11-17(20)22-14-15(2)13-19(4,5)6/h1
InchiKey: KKIANBFWNYWUBX-VAWYXSNFSA-N
Formula: C19H34O4
SMILES: CCCCCC(C)OC(=O)C=CC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-280.56	kJ/mol	Joback Method
hf	-827.18	kJ/mol	Joback Method
hfus	36.28	kJ/mol	Joback Method
hvap	74.09	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.670		Crippen Method
mcvol	289.150	ml/mol	McGowan Method
pc	1219.99	kPa	Joback Method
rinpol	2047.00		NIST Webbook
rinpol	2047.00		NIST Webbook
tb	786.75	K	Joback Method
tc	977.58	K	Joback Method
tf	415.55	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.41	J/mol×K	786.75	Joback Method
cpg	904.09	J/mol×K	818.55	Joback Method
cpg	920.76	J/mol×K	850.36	Joback Method
cpg	936.43	J/mol×K	882.16	Joback Method
cpg	951.16	J/mol×K	913.97	Joback Method
cpg	964.98	J/mol×K	945.77	Joback Method
cpg	977.93	J/mol×K	977.58	Joback Method
dvisc	0.0012707	Pa×s	415.55	Joback Method

dvisc	0.0004790	Pa×s	477.42	Joback Method
dvisc	0.0002259	Pa×s	539.28	Joback Method
dvisc	0.0001243	Pa×s	601.15	Joback Method
dvisc	0.0000765	Pa×s	663.02	Joback Method
dvisc	0.0000511	Pa×s	724.88	Joback Method
dvisc	0.0000364	Pa×s	786.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405606&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume